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Exploring divalent metal ion coordination. Unraveling binding modes in *Staphylococcus aureus* MntH fragments

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Streszczenie

Metal ion coordination is crucial in bacterial metabolism, while divalent metal ions serve as essential cofactors for various enzymes involved in cellular processes. Therefore, bacteria have developed sophisticated regulatory mechanisms to maintain metal homeostasis. These involve protein interactions for metal ion uptake, efflux, intracellular transport, and storage. *Staphylococcus aureus*, a member of the commensal flora, colonizes the anterior nares and skin harmlessly but can cause severe illness. MntH transporter is responsible for acquiring divalent metal ions necessary for metabolic functions and virulence. It is a 450-amino-acid protein analogous to Nramp1 (Natural Resistance-Associated Macrophage Protein 1) in mammals. Herein, the coordination modes of copper(II), iron(II), and zinc(II) ions with select fragments of the MntH were established employing potentiometry, mass spectrometry, and spectroscopic methods. Four model peptides, MNNKRHSTNE–NH_2, Ac-KFDHRSS–NH_2, Ac-IMPHNLYLHSSI–NH_2, and Ac-YSRHNNEE–NH_2, were chosen for their metal-binding capabilities and examined to determine their coordination properties and preferences. Our findings suggest that under physiological pH conditions, the N-terminal fragment of MntH demonstrates the highest thermodynamic stability with copper(II) and iron(II) ions. Furthermore, a comparison with other peptides from the *S. aureus* FeoB transporter indicates different binding affinities.

Słowa kluczowe

Staphylococcus aureus, MntH transporter, Metal-peptide complexes, Copper(II) complexes, Iron(II) complexes, Zinc(II) complexes

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